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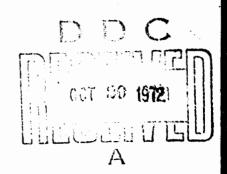


THEORY OF THE PHOTOFIELD EMISSION FROM METALS

bу

H. Neumann





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THEORY OF THE PHOTOFIELD EMISSION FROM METALS

[Article by Hans Neumann, Physics Department, Karl-Marx University, Leipzig; Leipzig, Annalen der Physik, German, Series 7, Vol 26, No 1, 1971, pp 89-93]

Summary

General relationships are developed for the field emission stream from a metal with simultaneous optical excitation. The influence of band structure on the energy distribution of the emitted electrons and the emission stream is discussed. Experimental results found for tungsten can be interpreted with qualitative accuracy.

1. Introduction

In a recently published paper [1] the photofield emission stream from a metal was deducted while completely neglecting band structure. The optical properties of the material were only taken into consideration by way of the quantity constants [2] gained with ordinary photoemission experiments. However, a comparison with experimental results for tungsten [3] shows that the experimental results cannot be described with this simple theory. This means, though, that the influence of band structure on the optical properties of the material may not be neglected. Therefore, it is the goal of this paper to develop relations for the emission stream which take into consideration the band structure.

2. Development of the Emission Equations

The density of the field emission stream is given in general form by the relation [4].

$$j = \frac{2c}{h^3} \int_{p_x = -\infty}^{+\infty} \int_{p_x = -\infty}^{+\infty} \int_{p_x = 0}^{\infty} F(E) D(E_x) \frac{\partial E}{\partial p_x} dp_x dp_y dp_z$$
 (1)

Here, q is the elementary charge, h is Planck's quantum of action, $\vec{p} = (p_x, p_y, p_t)$ the imputs of the electrons, E the total energy of the electrons, E_x the energy corresponding to the x-component of the impulse, $D(E_x)$ the penetration probability of the surface barrier, and F(E) the distribution function of the electrons. The x-direction is perpendicular to the emitter surface. If the Fermi level is chosen as zero of the energy count then the penetration probability of the surface barrier is

$$D(E_x) = \left[1 + \exp\left\{\frac{4\sqrt{2m}}{3q\hbar F}(\varphi - E_x)^{3/2}v\left(\frac{\sqrt{q^3F}}{\varphi - E_x}\right)\right\}\right]^{-1}.$$
 (2)

Here, m is the mass of the free electron, F the electric field applied from outside and φ the work function. The so-called Nordheim function v(y) can be found in tables [5, 6].

If polar coordinates are introduced into the plane which is perpendicular to the emission direction, and if $E = E_X + E_L$, then from equation (1) follows the relation

$$j = \frac{2mq}{k^3} \int_{E-E_a}^{\infty} F(E) dE \int_{\varphi=0}^{2\pi} d\varphi \int_{E_{\perp}=0}^{E_{\perp}^{\max}} D(E - E_{\perp}) dE_{\perp}.$$
 (3)

Ea is the lower edge of the conduction band.

The maximum value E_{\perp}^{\max} of E_{\perp} is a function of the total energy E and the polar angle φ and is determined by the band structure. In the case of simple band structures E_{\perp}^{\max} can be given explicitly in relation to E and φ [4].

With pure field emission without additional optical excitation, the integrals in equation (3) can be calculated since in that case $E_{\perp}^{\max} \approx E$, and the Fermi distribution is valid for the energy distribution of the electrons. In the following, we shall limit ourselves to the temperature T=0 K, from which it follows:

$$j_{F} = \frac{q^{2}F^{2}}{8\pi\hbar\varphi} \exp\left\{-\frac{4\sqrt{2m}}{3q\hbar F}\varphi^{3/2}v\left(\frac{\sqrt{q^{2}F}}{\varphi}\right)\right\}. \tag{4}$$

If, in addition the emitter is irradiated with light, then the energetic distribution F(E) of the electrons above the Fermi level is determined through optical excitation

processes. Consequently, to the pure field emission stream j_F a photo portion is added which results from the excited electrons. For this stream part j_P according to equation (3) is:

$$j_{P} = \frac{2mq}{\hbar^{2}} \int_{E=0}^{\infty} F(E) dE \int_{\varphi=0}^{2\pi} d\varphi \int_{E_{\perp}=0}^{E_{\perp}^{max}} D(E - E_{\perp}) dE_{\perp}.$$
 (5)

The energy distribution functions F(E) is connected with the optical properties and thus with the band structure of the material investigated it can be calculated in the following manner.

If it is assumed that each absorbed photon causes the excitation of an electron, then the number of the electrons excited in the distance z from the surface in a layer of thickness dz into the energy interval E... E + dE above the Fermi level is equal to

$$q(E, \varepsilon, z) dE dz = [1 - R(\varepsilon)] N(\varepsilon) \exp\{-\alpha(\varepsilon) z\} \alpha'(E, \varepsilon) dE dz.$$
 (6)

 $N(\epsilon)$ is the number of photons hitting the surface with the energy ϵ , $R(\epsilon)$ the reflection coefficient, $\alpha(\epsilon)$ the absorption coefficient for photons of the energy ϵ , and $\alpha'(E,\epsilon)$ is the absorption coefficient for the excitation of electrons in the energetic state E through photons of the energy ϵ . Of these electrons only a certain part y(E, z) will arrive at the surface, since scattering processes on the path to the surface lead to ϵ reduction of the electron energy. In good approximation these processes can be described through a damping length L(E) [7], so that

$$y(E, z) \approx \exp\{-z/L(E)\}$$
 (7)

If (7) is inserted in (6) then after integrating over z one obtains the number of the electrons with energies between E and E + dE which are present at the surface during excitation with photons of the energy ε

$$q(E,\varepsilon) dE = [1 - R(\varepsilon)] \dot{N}(\varepsilon) \alpha'(E,\varepsilon) \left[\alpha(\varepsilon) + \frac{1}{L(E)}\right]^{-1} dE.$$
 (8)

If excitation does not take place with photons of one single energy but over a certain spectral region, then one still has to integrate over the photon energies. Thus we have the following expression for the energy distribution F(E)

$$F(E) dE = \int [1 - R(e)] N(e) \alpha'(E, e) \left[\alpha(e) + \frac{1}{L(E)} \right]^{-1} de dE.$$
 (9)

The connection of the distribution function with the band structure is supplied by way of the material magnitudes $R(\varepsilon)$, α (ε) and $\alpha'(E,\varepsilon)$.

In the following, it is assumed that the reflection coefficient is only weakly dependent on the photon energy. Also, the influence of $\alpha(\epsilon)$ on the distribution function will be small since the damping length L(E) is of the order of magnitude of 10^{-6} cm [7], so that $\alpha(\epsilon) \lesssim 1/L(E)$. It follows then, that the considerable influence of the band structure on the distribution function F(E) is due to the absorption coefficient $\alpha'(E,\epsilon)$.

For the absorption coefficient $\alpha'(E, \epsilon)$ we have [8]

$$\alpha'(E,\varepsilon) := \frac{\pi^2 e^2 E^2}{\pi^2 e^2} r(E,\varepsilon). \tag{10}$$

where $r(E, \epsilon)$ represents the number of the induced transitions into the energy level E. From the Dirac disturbance theory follows [8]

$$\tau(\mathbf{f},\varepsilon) d\mathbf{f} d\varepsilon = \frac{4q^3\varepsilon^2n}{3m^2c^3\hbar^2} \varrho(\mathbf{f}) \int_{\mathbf{f}_0} \varrho_0(\mathbf{f}_0) |P_{\mathbf{f}_0}|^2 \delta(E - E_0 - \varepsilon) d\mathbf{f}_0 d\mathbf{f} d\varepsilon. \qquad (11)$$

Here, n is the index of refraction, c the speed of light, $\varrho(t)$, t and E, density state, the wave number vector, and the energy of the final state, $\varrho_0(t_0)$, t_0 and E_0 are the corresponding magnitudes of the initial state of the electrons taking part in the transition. P_{t_0} is the matrix element of the transition. With further consideration of equation (11) one has to differentiate between direct transitions (k-conservation) and indirect transitions (random k-combinations). If $r(E,\varepsilon)$ is calculated for these two cases in the usual manner [8], inserted in (10) and then integration carried out in equation (9) one obtains in the case of direct transitions

$$F_{d}(E) dE = \frac{\pi^{2}q^{2}h}{cnm^{2}} (1 - R) \left[\alpha + \frac{1}{L(E)} \right]^{-1} \times N(E - E_{0}) \varrho(E) \varrho_{0}(E_{0}) \frac{|P_{\pi}|^{2}}{k^{2}} \left(\frac{\partial(E - E_{0})}{\partial|k|} \right)^{-1} dE.$$
(12)

For indirect transitions we have

$$F_{\text{lad}}(E) dE = \frac{n^2 q^2 \hbar}{cnm} (1 - R) \left[\alpha + \frac{1}{L(E)} \right]^{-1} \times \varrho(E) \int |P_{R_0}|^2 \varrho_0(E - \varepsilon) N(\varepsilon) d\varepsilon dE.$$
(13)

Now it is possible to calculate with the aid of equations (12), (13), and (5) the photo share of the field emission stream if matrix elements, state densities, and E(t)- slopes are known.

3. Discussion

It follows from the relationships developed that the band structure becomes noticeable in two ways in the photofield emission stream. For one, the distribution function of the optically excited electrons (equations (12) and (13)) is influenced, for another the maximum value of E_{\perp} in equation (5) is determined through the E(t) slope. It is not easy to say whether one of the two factors predominates. It is likely that the absorption coefficient exerts the dominating influence. For this reason it is assumed below that the influence of the band structure on E_{\perp}^{\max} can be neglected in first approximation and that as in the case of pure field electron emission E_{\perp}^{\max} can be set $\approx E$.

$$G(E, F) = \int_{E_{\perp}=0}^{E} D(E - E_{\perp}) dE_{\perp}$$
 (14)

can be calculated numerically as a function of E and F by taking into consideration (2). Fig. 1 shows the result of the calculation.

The total-energy distribution P(E) dE of the emitted electrons are found from (5), (12) and (13) to be

$$P_d(E) dE \sim N(E - E_0) \varrho(E) \varrho_0(E_0) \frac{|P_R|^2}{k^2} \left(\frac{\partial (E - E_0)}{\partial |k|}\right)^{-1} G(E, F) dE$$
 (15)

for direct transitions and

$$P_{\text{ind}}(E) dE \sim \varrho(E) G(E, F) \int |P_{\text{tt}}|^2 \varrho_0(E - \varepsilon) N(\varepsilon) d\varepsilon dE$$
 (16)

for indirect transitions. Here, all constant factors were omitted. Taking into consideration Fig. 1 it follows from equations (15) and (16) that the energy distribution of the electrons emitted changes only little with the field

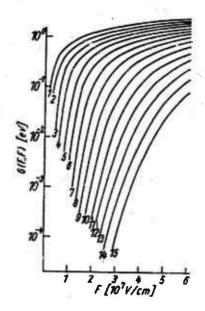


Fig 1. Calculated Curves for the Integral G(E,F) as a Function of F with E as Parameter (curve 1:

E=4,0 eV, 2:3,8 eV, 3:3,6 eV, 4:3,4 eV, 5:3,2 eV, 6:3,0 eV, 7:2,8 eV, 8:2,6 eV, 9:2,4 eV, 10:2,2 eV, 11:2,0 eV, 12:1,8 eV, 13:1,6 eV, 14:1,4 eV, 15:1,2 eV)

strength at the field strengths of $2 \times 10^7 \dots 6 \times 10^7$ V/cm which are typical for the field electron emission at high electron energies (2.6 eV and more above the Fermi level). Clearly defined changes in the energy distribution can be expected for energies below 2 eV. From this, conclusions can be drawn on the behavior of the field emission stream with optical excitation.

Intensive optical transitions to high energies will result in a relatively large photofield emission which is only slightly changeable with the outside field. However, if intensive optical transitions in energy levels of 1.2... 1.0 eV above the Fermi level are present, a stream can be expected which increases quickly with the outside field.

If this result of the general theory is compared with the experimental results [3] obtained for tungsten, the conclusion is arrived at that intensive transitions to high as well as to low energies have to be present. The

stream remains almost constant to field strengths of about $3...4 \times 10^7$ V/cm and then rises very steeply. Comparing the experimental curves with Fig. 1, it can be concluded that for this steep rise a transition into an energy level between 1.2 eV and 1.6 eV above the Fermi level has to be responsible. This result agrees with the theoretically calculated band structure given by Mattheiss [9]. According to [9] a direct transition to E = 1.45 eV above the Fermi level with an excitation energy of about 2.9 eV can be expected.

Thus, the experimental results of the photofield emission from tungsten have been interpreted qualitatively. Extensive numerical calculations under consideration of the state densities will be published in the future in connection with a summary presentation of the experimental results.

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